

## FOURIER TRANSFORM INFRARED STUDIES OF COAL STRUCTURE

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In the 1950's and 1960's infrared spectroscopy was a widely used analytical tool for characterizing the structure of coal. It was recognized that the infrared spectrum contained information concerning aliphatic and aromatic hydrogen, hydroxyl groups and carbonyls, to mention those functional groups whose bands are most easily assigned and measured. Unfortunately, quantitative measurements were complicated first by the overlap of the broad bands characteristic of a multi-component macromolecular system, and second by the questions concerning measurements of extinction coefficients. These are elusive parameters relating the intensities of specific bands to the concentration of the corresponding functional groups. Partly because of these difficulties the use of infrared spectroscopy was in decline by the early 1970's and other techniques (e.g., NMR) came to the fore.

This general decline in the use of infrared spectroscopy has recently been reversed with the introduction of Fourier transform instruments. Although these instruments have various optical advantages over dispersive spectrometers, the most significant advances have occurred through the use of the dedicated on-line minicomputer that is an integral part of the system. Programs capable of a range of manipulations, such as spectral subtraction, baseline straightening, curve resolving and factor analysis can now be routinely applied. Naturally, this type of analysis is not unique to FT-IR and many programs and techniques that are applicable to coal studies were developed in the 1960's for use with (often laboriously obtained) digitized data. These methods can now be routinely and easily applied. However, this in itself produces problems, since the uncritical application of complex programs can result in serious error. Judgement is still required of the spectroscopist and infrared spectroscopy remains something of an art.

In this presentation the problems associated with applying computer methods will be considered, with particular reference to the determination of hydrogen containing functional groups. The difficulties associated with the determination of extinction coefficients still remain and the methods now being used, model compounds, equating appropriate bands to measurements of elemental hydrogen, and calibration using soluble extracts and proton magnetic resonance, were in fact first developed in the 1960's. Values obtained using the data handling capabilities of FT-IR instruments will be considered and compared to previously reported results. These parameters have been applied to a set of vitrinite concentrates and the determination of structural parameters by combining FT-IR and  $^{13}\text{C}$  NMR measurements will be considered.